

Generation and Application of Problem Specific Property Models in Process Design

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Property models play distinct but different roles in process design and analysis. They play a service role if they provide property values only when requested as in typical process simulation problems. They play a service/advice role if in addition to providing the requested property values, they also indicate the infeasible design alternatives as in the case of generation and screening of process flowsheet alternatives. Property models may also play a service/advice/solve role where in addition to the above roles, they also help to reformulate the design problem so that more simpler, efficient and visual solution techniques can be developed. Graphical design techniques typically employ property models in this role.

The different roles of property models means that it is important to select the appropriate model for a specified design problem. Improper selection may lead to qualitative as well as quantitative errors in the solution of the design problem. Also, it should be noted that in process design, different types of "problem specific" property models may be needed. These problem specific models can be generated from a general property model framework that is based on the identification of the specific needs design/analysis problem.

The objective of this paper is to highlight the property needs in process design, the generation of the corresponding problem specific models and finally, to provide an efficient/reliable application of the property model for the solution of process design/analysis problems. A wide range of processes, handling hydrocarbon systems, electrolyte systems and complex (multifunctional) compounds will be used to illustrate various features of the property model framework.

Finally, generation/use of different versions of property models from a reference model will be highlighted for the same process but at different stages of its life cycle.